Pentanedioic acid, hexafluoro-376-73-8 | DTXSID8059926

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 4.72 days

Global applicability domain: Outside

Local applicability domain index: 3.11e-01

Confidence level: 7.70e-01

Nearest Neighbors from the Training Set

Image not found

Propylbenzene Measured: 24.3 Predicted: 4.02 Image not found

Tetradeca-1,13-diene Measured: 367 Predicted: 8.69 Image not found

2-Methylhexane Measured: 12.5 Predicted: 5.54

Image not found

2-Methylheptane Measured: 12.5 Predicted: 3.99 Image not found

2-Methyloctane Measured: 40.7 Predicted: 4.23